

Supporting Information

AIE-ligand-based luminescent Cd(II)-organic framework as the first “turn-on” Fe³⁺ sensor in aqueous medium

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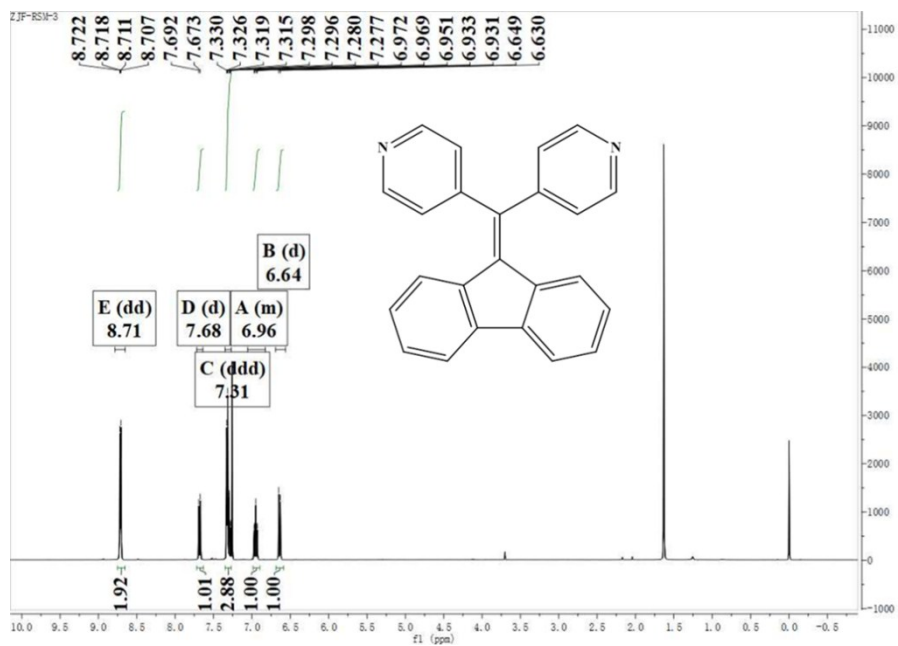


Fig. S1 ^1H NMR spectroscopy of **L**.

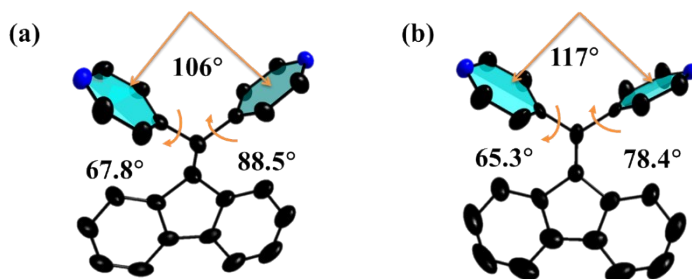


Fig. S2 (a) the single crystal structure of **L**; (b) the structure of **L** in MOF **1**.

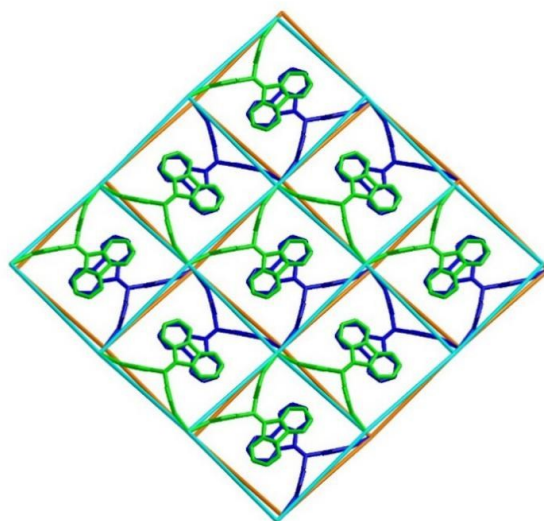


Fig. S3 The overlap of the fluorene ring (part of atoms from H₂NDA and **L** are omitted for clarity).

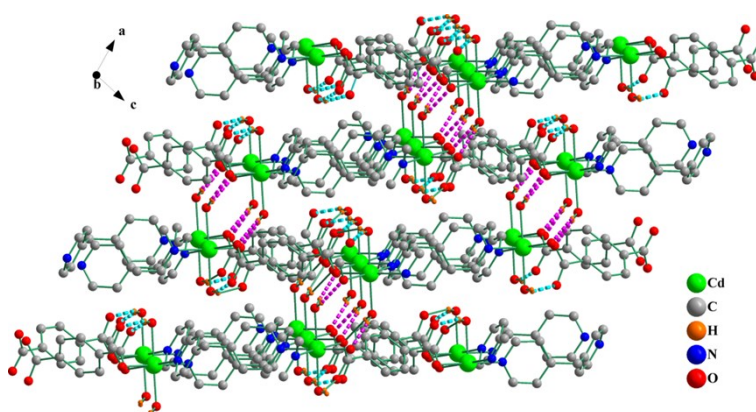


Fig. S4 The 3-D supramolecular framework of **1**.

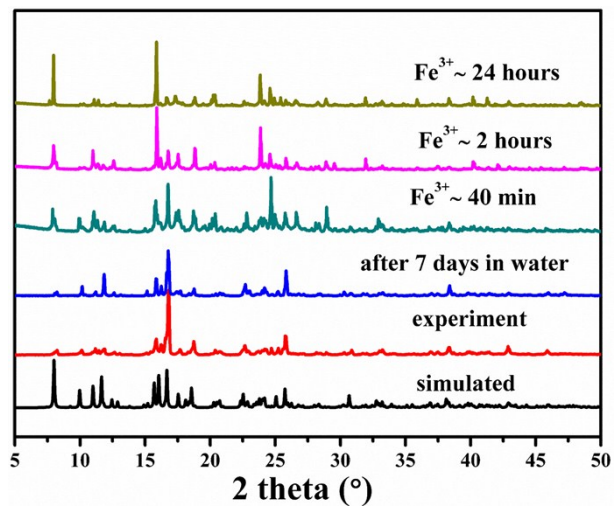


Fig. S5 The PXRD of 1.

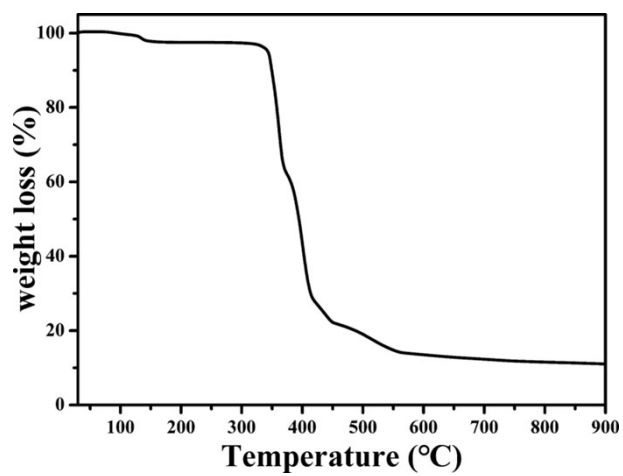


Fig. S6 The TGA of 1.

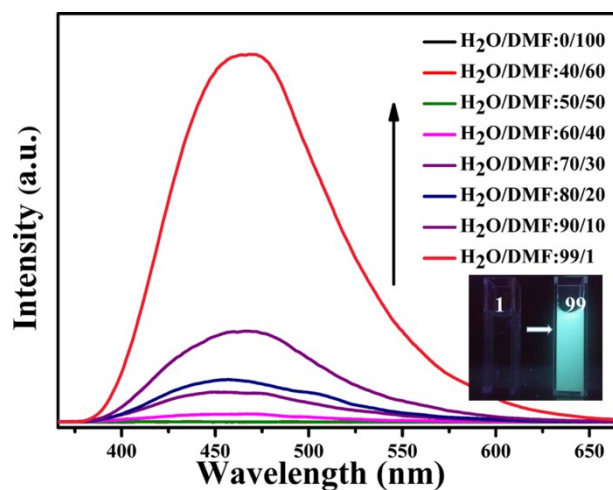


Fig. S7 Photoluminescence (PL) spectra of **1** in DMF/water mixture with various water fractions (f_w).

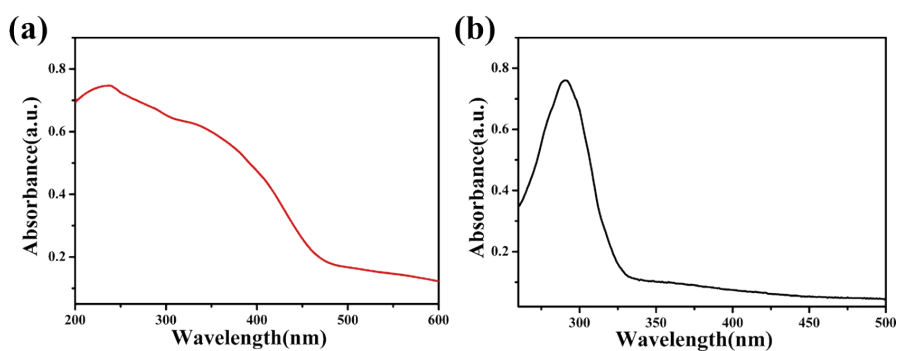


Fig. S8 The UV-vis absorption spectra of **1** (a) in solid state; (b) aqueous medium.

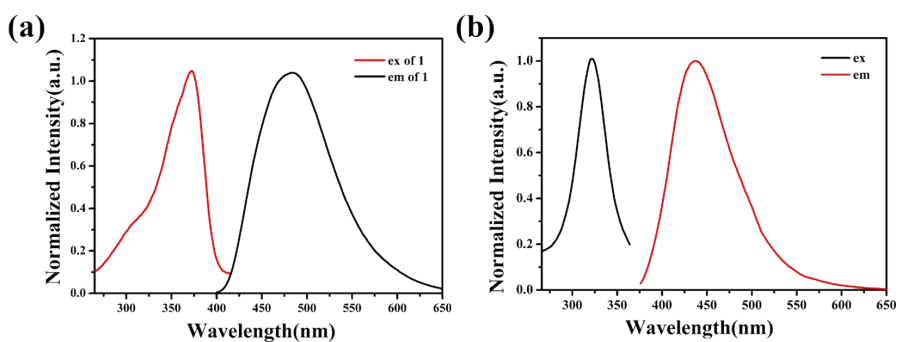


Fig. S9 (a) The solid excitation and emission spectra of **1**; (b) the excitation and emission spectra of the water suspensions of **1**.

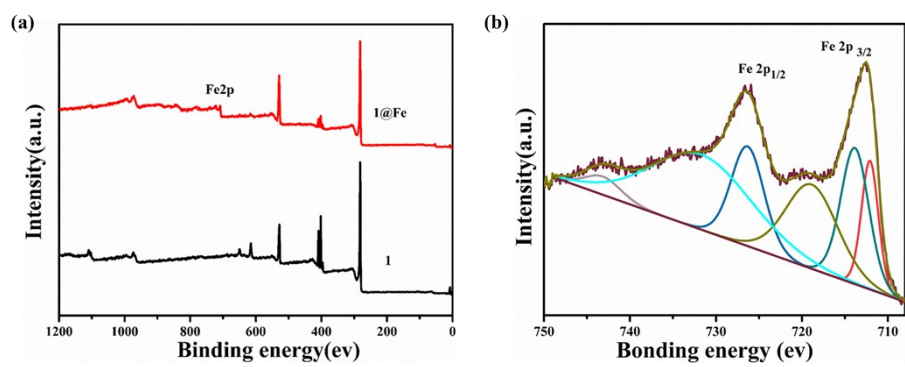


Fig. S10 (a) The XPS of **1** and **1@Fe**; (b) Fe 2p spectra of **1@Fe**.

Table S1 Selected bond lengths (Å) for **1**

Compound 1			
Cd(1)-O(6)#1	2.3078(17)	Cd(1)-O(1)	2.320(2)
Cd(1)-N(1)	2.324(2)	Cd(1)-O(3)	2.3249(17)
Cd(1)-O(2)	2.339(2)	Cd(1)-N(2)	2.352(2)
#1 -x, y+1/2, -z+1/2	#2 -x+1, y-1/2, -z+3/2		
#3 -x, y-1/2, -z+1/2	#4 -x+1, y+1/2, -z+3/2		

Table S2 Selected angles (°) for **1**

Compound 1			
O(6)#1-Cd(1)-O(1)	91.42(7)	O(6)#1-Cd(1)-N(1)	99.22(7)
O(1)-Cd(1)-N(1)	92.89(7)	O(6)#1-Cd(1)-O(3)	86.74(6)
O(1)-Cd(1)-O(3)	85.69(7)	N(1)-Cd(1)-O(3)	173.91(6)
O(6)#1-Cd(1)-O(2)	93.87(7)	O(1)-Cd(1)-O(2)	173.55(8)
N(1)-Cd(1)-O(2)	89.90(8)	O(3)-Cd(1)-O(2)	90.93(7)
O(6)#1-Cd(1)-N(2)	170.97(7)	O(1)-Cd(1)-N(2)	88.12(8)
N(1)-Cd(1)-N(2)	89.81(7)	O(3)-Cd(1)-N(2)	84.23(7)
O(2)-Cd(1)-N(2)	86.07(8)		
#1 -x, y+1/2, -z+1/2	#2 -x+1, y-1/2, -z+3/2		
#3 -x, y-1/2, -z+1/2	#4 -x+1, y+1/2, -z+3/2		

Table S3 Selected H-bond lengths (Å) for **1**

Compound 1					
Donor – H	Acceptor	D – H	H ⋯ A	D ⋯ A	D – H ⋯ A
O1 – H3	O3	0.82	1.87	2.6424	157
O1 – H7	O6	0.86	2.07	2.8617	153
O2 – H8	O5	0.86	1.82	2.6595	165
O2 – H9	O4	0.74	1.96	2.6553	158